

Interpolation of MODFLOW flux onto a piecewise linear surface

Carl W. Gable, Terry Cherry
EES-6 Hydrology, Geochemistry and Geology
Los Alamos National Laboratory

1.0 Overview

The goal of this project is to develop a method to interpolate output from a MODFLOW saturated zone calculation onto an arbitrary surface in order to apply boundary conditions to a model whose domain is fully embedded in the domain of the MODFLOW model but is not aligned with the MODFLOW grid. This method is demonstrated with a specific application interpolating from the NTS-UGTA Regional Groundwater MODFLOW model onto a vertical plane in Western Pahute Mesa. The MODFLOW model is rotated 5 degrees. The vertical plane onto which fluxes are interpolated is along an east-west transect. The interpolated flux across the plane is $0.952\text{E}+03 \text{ m}^3/\text{day}$.

2.0 Method

The need to compute flux values on surfaces which are not coincident with the cell boundaries of a MODFLOW model can arise when one wishes to use the results of a large scale MODFLOW calculation as boundary conditions for a smaller scale calculation. If the small scale calculation is perfectly coincident with the grid cells of the MODFLOW model, it is relatively easy to add all flux values on the shared boundary to obtain a flux boundary condition. If the small scale calculation is not coincident with the grid cells of the MODFLOW model, it is necessary to develop a method to interpolate from the MODFLOW results onto the boundary. For many models, the surface upon which boundary conditions are applied is a plane, however the methods developed for this project are not limited to interpolating on a plane. More general surfaces, which can be defined by a collection of triangular elements, are supported in this method. This provides a general capability for computing flux across simple planar surfaces or more geometrically complex surfaces.

2.1 Method Details

Output from MODFLOW defines the flux out of the six sides of each grid cell. In addition there are terms for sources and sinks. To interpolate this to a continuous function defined anywhere within the domain there are a number of assumptions made about the form of the MODFLOW output and the desired result. The MODFLOW flux is defined on each face of a rectangular control volume. Opposite faces are parallel and have equal area. We

assume that the flux across any surface parallel to a pair of faces but contained within the control volume is a linear combination of the flux values on the faces. This is analogous to the methods used to obtain velocities within orthogonal MODFLOW cells for particle tracking. There may be some cells associated with sources or sinks such that the sum of all face fluxes are not zero but this does not pose any problem to the interpolation method.

The surface across which flux is interpolated from the MODFLOW model must be a piecewise linear surface. It can be a plane or it can be a triangulation made up of a collection of triangles. The triangles do not have to share edges and can be disjoint. A triangulation should be fully contained within the MODFLOW domain or coincident with the MODFLOW boundary. If there are triangles that are partly inside and partly outside errors will be introduced. If the surface is coincident with MODFLOW cell boundaries the method will produce a result that is exactly equal to the sum of the MODFLOW cell face fluxes. If the surface is a closed surface and the MODFLOW calculation has no sources or sinks, the flux calculation will compute a net flux through the surface of zero. If there are sources or sinks, the flux will be the sum of the source terms contained within the closed surface.

From an operational point of view, the approach makes some assumptions and converts the flux information into an approximation of Darcy velocity. All interpolation and integration calculations take place on the velocity field. We assume velocity is constant on each face and is orthogonal to faces. Velocity varies linearly within MODFLOW cells and has discontinuous derivative at cell boundaries. The approximation assures that the integral of velocity over a MODFLOW cell face will be the MODFLOW flux.

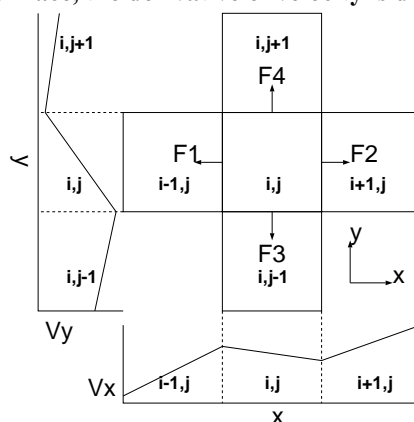
The flux across any arbitrary surface is defined as, $F = \int_S V \cdot \hat{n} dS$, where V is the velocity vector field, \hat{n} is the normal vector to the surface and dS is a surface element. The output from MODFLOW is in the form of six flux values for each control volume, $F_1, F_2, F_3, F_4, F_5, F_6$. The units of flux are cubic meters per day with the convention that positive flux is into a cell and negative flux is out of a cell. Flux is converted to Darcy velocity perpendicular to each face assuming the velocity is constant over each face and, $V_i = F_i / A_i \cdot n_i$, where A_i is the area of a control volume face and \hat{n} is the outward normal to the cell face. The velocity on the faces is zero parallel to the control volume faces and varies linearly in the direction normal to the faces as the cell is traversed from one cell face to another. The form of the velocity within a cell is,

$$V(x, y, z) = [a(F_1, F_2)x + b(F_1, F_2)]\hat{x} + [c(F_3, F_4)y + d(F_3, F_4)]\hat{y} + [e(F_5, F_6)z + f(F_1, F_2)]\hat{z}$$

This representation uses the six flux values to represent the velocity in terms of six unknowns. The x, y, z components of velocity are only a function of their respective coordinate (Figure 1). The velocity component normal to a face is continuous as a cell face is

crossed, the derivative is discontinuous. The velocity parallel to a cell face may be discontinuous when a cell face is crossed. We then have at our disposal a representation of the velocity field within each cell in terms of three velocity components that vary linearly. The next step is to interpolate these velocity components onto a piecewise linear surface cutting through the 3D MODFLOW grid.

FIGURE 1. Schematic representation of velocity on a 2D grid. x velocity is only a function of x , y velocity is only a function of y . Velocity varies linearly inside a grid cell. Velocity normal to a cell face is continuous across a cell face, the derivative of velocity is discontinuous.



There are limits to the type of piecewise linear surface over which the method will integrate the flux accurately. The surface must have boundaries that are inside or on the boundaries of the 3D MODFLOW grid. The surface cannot extend outside the 3D grid or errors will be introduced. In addition, the facets of the surface must be coincident with the cell boundaries of the 3D grid. This criteria is easily met if the surface is created with the ‘extract’ command which is part of LaGriT. This operation will intersect a surface with a 3D grid of hexahedra and compute the geometry and topology of the intersection surface with the edges of the 3D grid. The result is a topologically 2D object in 3D space (Figure 2). The intersection may be composed of quadrilateral and triangular elements but another LaGriT command, `quadtotri`, converts the surface into all triangular elements. If these criteria are not met the method will still provide a solution but errors are introduced.

LaGriT interpolation routines are used to interpolate the velocity components defined on nodes of the 3D grid onto all the nodes of the 2D surface grid (Figure 3). The result is a triangulated surface with three velocity components on each triangle vertex. The flux across the surface is then the integral of the velocity component normal to each triangle facet. New features developed for this project include the ability to take dot products of vector attributes on a grid, computation of area normal vectors as attributes of a triangle mesh and integration of a scalar function over a triangular surface.

It is assumed that the velocity varies linearly on the triangle elements. The normal component of velocity is integrated over each triangle and stored in an element based array. The total flux is then the sum of all the flux on each triangle. This is computed using the LaGriT ‘math’ function which allows one to sum a set of element or node array values into a scalar.

All the computational infrastructure to perform the computations described have been implemented within the LaGriT (www.t12.lanl.gov/~lagrit) software package.

FIGURE 2. The plane over which flux is integrated is shown embedded inside a small piece of the MODFLOW grid. The quantity plotted on the plane is flux in m^3/day .

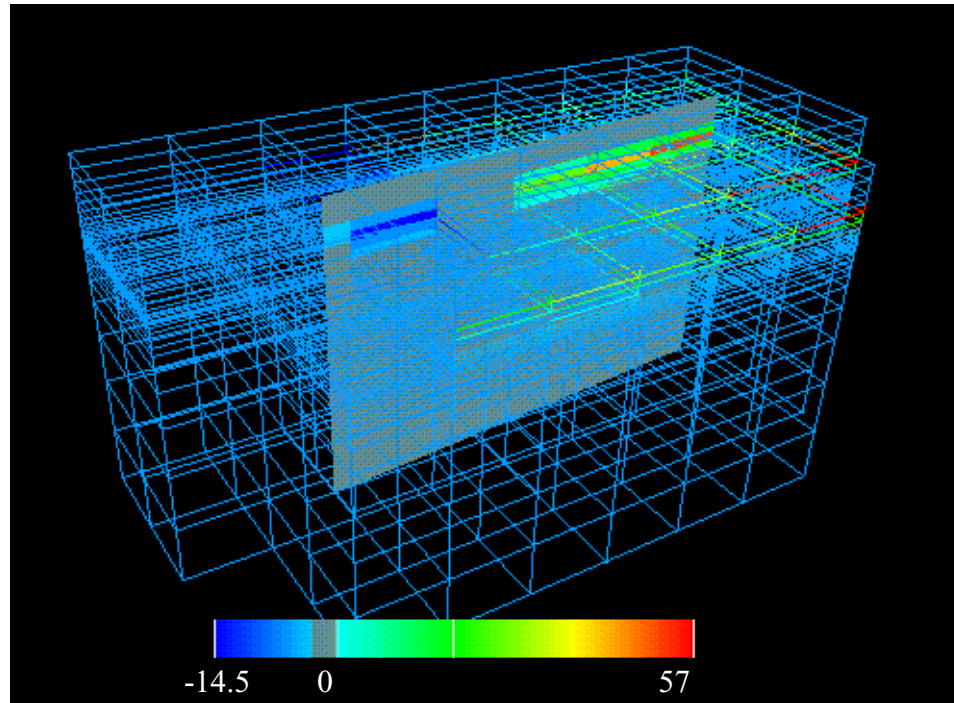
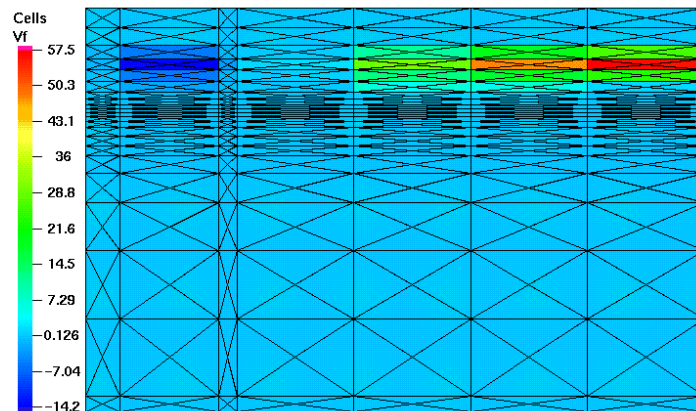


FIGURE 3. The flux (m^3/day) on each subtriangle on the plane of interest. The narrow column on the left side result from the place where the transect cuts across a corner of one of the MODFLOW cells. The sum of the flux on each triangle is the total flux across this surface.



3.0 Result

Output from a MODFLOW calculation is used as input. The MODFLOW results are reported in units of m^3/day .

For this application the surface through which flux is computed is defined by a planar quadrilateral with four sets of x, y, z coordinates (see Figure 4, Figure 5). The coordinates which define the plane are;

```
0.5431560E+06 0.4125121E+07 -0.3200000E+04
0.5511560E+06 0.4125121E+07 -0.3200000E+04
0.5511560E+06 0.4125121E+07 0.2000000E+04
0.5431560E+06 0.4125121E+07 0.2000000E+04
```

The total area of this plane is: $0.416\text{E}+08 \text{ m}^2$

The total volume/time across this plane is: $0.952\text{E}+03 \text{ m}^3/\text{day}$

The integrated flux is also calculated to a depth of $-0.40\text{E}+4$, which is the bottom of the MODFLOW grid. In that case:

```
0.5431560E+06 0.4125121E+07 -0.4000000E+04
0.5511560E+06 0.4125121E+07 -0.4000000E+04
0.5511560E+06 0.4125121E+07 0.2000000E+04
0.5431560E+06 0.4125121E+07 0.2000000E+04
```

The total area of this plane is: $0.480\text{E}+08 \text{ m}^2$

The total volume/time across this plane is: $0.952\text{E}+03 \text{ m}^3/\text{day}$

Note that the cubic meters per day calculation does not change, to within five significant figures, with a change in the depth of the surface. This is because the flux across the bottom portion of the plane is very small.

The results reported are strongly influenced by a small number of cells with large flux values. The majority of the cells in the region around the plane of interest have horizontal flux values close to zero. There is some canceling because there is flow in both the positive direction and the negative direction.

FIGURE 4. The MODFLOW grid viewed from above.

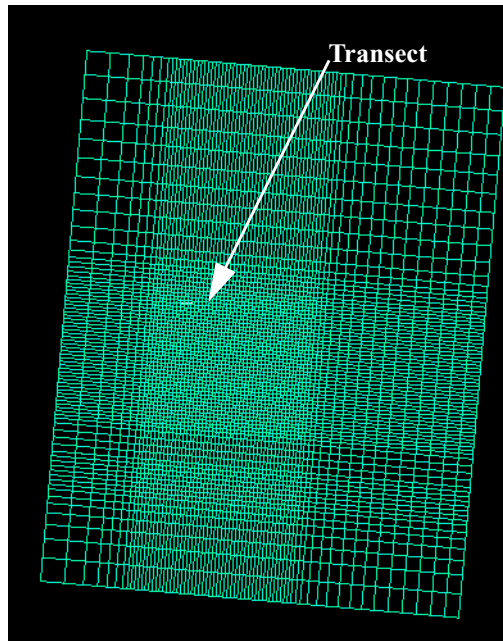
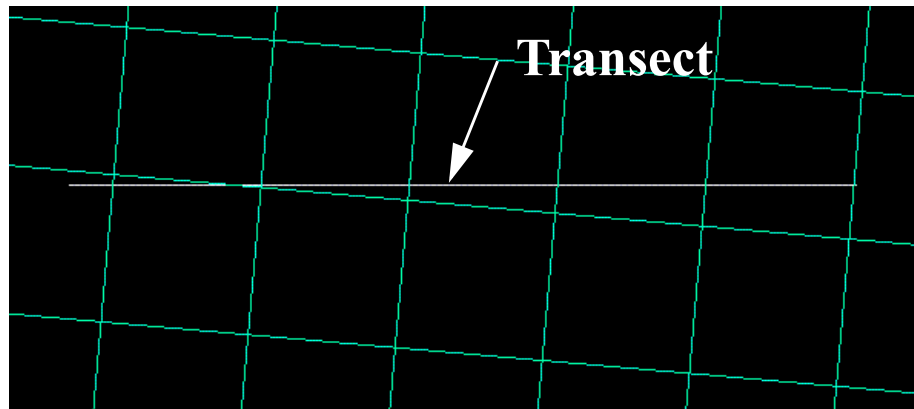


FIGURE 5. A close-up of the transect over which flux is calculated. Note that transect does not exactly align with MODFLOW cells. Integration method computes the fractional flux where the transect ends within the cell.



4.0 Appendix

A detailed description of each step in the process, all data files and LaGriT control files and additional graphics, can be found in the HTML archive,

ees-www.lanl.gov/EES5/geomesh/catalogue/NTS_MODFLOW_FLUX/catalog.html